

The calculation of the thermal properties of graphene under a magnetic field via the two-dimensional Dirac oscillator

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Abstract

In this paper, we show, by using the approach of effective mass, that the model of a two-dimensional Dirac oscillator can be used to describe the thermal properties of graphene under an uniform magnetic field. All thermal quantities of graphene, such as the free energy, the mean energy, the entropy and the specific heat, have been found by using an approach based on the zeta function.

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I. INTRODUCTION

Graphene is a two-dimensional configuration of carbon atoms organized in a hexagonal honeycomb structure. The electronic properties of graphene are exceptionally novel. For instance, the low-energy quasi-particles in graphene behave as massless chiral Dirac fermions which has led to the experimental observation of many interesting effects similar to those predicted in the relativistic regime. Graphene also has immense potential to be a key ingredient of new devices, such as single molecule gas sensors, ballistic transistors and spintronic devices.

The Dirac relativistic oscillator is an important potential both for theory and application. It was for the first time studied by Ito et al [2]. They considered a Dirac equation in which the momentum \vec{p} is replaced by $\vec{p} - im\beta\omega\vec{r}$, with \vec{r} being the position vector, m the mass of particle, and ω the frequency of the oscillator. The interest in the problem was revived by Moshinsky and Szczepaniak [3], who gave it the name of Dirac oscillator (DO) because, in the non-relativistic limit, it becomes a harmonic oscillator with a very strong spin-orbit coupling term. Physically, it can be shown that the (DO) interaction is a physical system, which can be interpreted as the interaction of the anomalous magnetic moment with a linear electric field [4, 5]. The electromagnetic potential associated with the DO has been found by Benitez et al [6]. The Dirac oscillator has attracted a lot of interest both because it provides one of the examples of the Dirac's equation exact solvability and because of its numerous physical applications (see Ref [7] and references therein). Recently, Franco-Villafane et al [8] exposed the proposal of the first experimental microwave realization of the one-dimensional DO. The experiment relies on a relation of the DO to a corresponding tight-binding system. The experimental results obtained, concerning the spectrum of the one-dimensional DO with and without the mass term, are in good agreement with those obtained in the theory. In addition, Quimbay et al [9, 10] show that the Dirac oscillator can describe a naturally occurring physical system. Specifically, the case of a two-dimensional Dirac oscillator can be used to describe the dynamics of the charge carriers in graphene, and hence its electronic properties. Also, the exact mapping of the DO in the presence of a magnetic field with a quantum optics leads to regarding the DO as a theory of an open quantum systems coupled to a thermal bath [11].

The particle effective mass in graphene is a challenging concept because the commonly

used theoretical expression is mathematically divergent. Ariel et al [12, 13] use a basic principles to present a simple theoretical expression for the effective mass that is suitable for both parabolic and non-parabolic isotropic materials such as graphene. In particular, they demonstrate that the definition of effective mass is consistent with the definition of the cyclotron effective mass, which is one of the common methods for effective mass measurement in solid state materials, and consequently their proposed definition of the effective mass can be used for non-parabolic materials such as graphene.

In this article, we attempt to introduce the Dirac oscillator interaction for describing the electronic properties of graphene in an external magnetic field, by using the concept of the effective mass. This model leads to the relativistic dispersion relation observed for graphene, and explain the existence of a chiral phase transition. Also, it allows us to investigate the thermodynamic properties of graphene in the presence of a constant magnetic field. In particular, we determined the behavior of the main thermodynamical functions: the free energy, the mean energy, the entropy and the specific heat.

This work is outlined as follows. In Sec. II, we expose our approach concerning the introduction of the Dirac oscillator interaction by using the formalism of the effective mass in graphene: in this case, the eigensolutions have been obtained by using the formalism of a complex (two-dimensional) quantum relativistic harmonic oscillator. In Sec. III, the all thermodynamic quantities that describe the thermal physics of graphene have been calculated via an approach based on zeta function. Finally, in sec. IV, we present the conclusion.

II. EIGENSOLUTIONS OF GRAPHENE VIA A TWO-DIMENSIONAL MASS-LESS DIRAC OSCILLATOR

A. complex formalism

In terms of complex coordinates and its complex conjugate [14] , we have

$$z = x + iy, \bar{z} = x - iy, \quad (1)$$

and

$$\frac{\partial}{\partial z} = \frac{1}{2} \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right), \frac{\partial}{\partial \bar{z}} = \frac{1}{2} \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right). \quad (2)$$

The operators momentum p_x and p_y , in the Cartesian coordinates, are defined by

$$p_x = -i\hbar \frac{\partial}{\partial x}, p_y = -i\hbar \frac{\partial}{\partial y}. \quad (3)$$

When we use $p_z = -i\hbar \frac{\partial}{\partial z}$, we get

$$p_z = -i\hbar \frac{d}{dz} = \frac{1}{2} (p_x - ip_y), \quad (4)$$

$$\bar{p}_z = -i\hbar \frac{d}{d\bar{z}} = \frac{1}{2} (p_x + ip_y), \quad (5)$$

with $p_z = -\bar{p}_z$. These operators obey the basic commutation relations

$$[z, p_z] = [\bar{z}, p_{\bar{z}}] = i\hbar, [z, p_{\bar{z}}] = [\bar{z}, p_z] = 0. \quad (6)$$

The usual creation and annihilations operators, a_x and a_y with

$$a_x = \sqrt{\frac{m\omega}{2\hbar}} x + i \frac{1}{\sqrt{2m\omega\hbar}} p_x, a_y = \sqrt{\frac{m\omega}{2\hbar}} y + i \frac{1}{\sqrt{2m\omega\hbar}} p_y, \quad (7)$$

can be reformulated, in the formalism complex, as follows

$$a_z = i \left(\frac{1}{\sqrt{m\omega\hbar}} \bar{p}_z - \frac{i}{2} \sqrt{\frac{m\omega}{\hbar}} z \right), \quad (8)$$

$$\bar{a}_z = -i \left(\frac{1}{\sqrt{m\omega\hbar}} p_z + \frac{i}{2} \sqrt{\frac{m\omega}{\hbar}} \bar{z} \right). \quad (9)$$

These operators, also, satisfy the habitual commutation relations

$$[a, \bar{a}_z] = 1, [a, a] = 0, [\bar{a}_z, \bar{a}_z] = 0. \quad (10)$$

B. The framework theoretical of a two-dimensional Dirac oscillator

We start with the free massive Dirac equation

$$i\hbar \frac{\partial \psi}{\partial t} = H_D \psi, \quad (11)$$

where the wave function $\psi = \begin{pmatrix} \psi_1, \psi_2 \end{pmatrix}^T$ in the graphene case describes the electron states around the Dirac point K and K' , and the Dirac Hamiltonian is given by

$$H_D = c\vec{\alpha} \cdot \vec{p} + \beta mc^2, \quad (12)$$

where $\vec{\alpha}$ and β are the Dirac matrices.

In the case of graphene, one has massless particles that move through the honeycomb lattice with a velocity $\tilde{c} \sim 1.1 \times 10^6 \text{ms}^{-1}$ [17], the so-called Fermi velocity. Thus, E. (12) reads

$$H_D = \tilde{c}\vec{\alpha} \cdot \vec{p}. \quad (13)$$

Now, the introduction of the Dirac oscillator interaction in graphene can be made by using the model of the effective mass m^* as follows: the momentum operator \vec{p} , in E. (13), could be substituted by $\vec{p} - im^*\omega\vec{r}$, where the additional term is linear in r , and m^* is the effective mass. In this case, E. (11) becomes

$$[\tilde{c}\sigma_x(p_x - im^*\omega x) + \tilde{c}\sigma_y(p_y - im^*\omega y)]\psi = E\psi. \quad (14)$$

With the following definitions of Dirac matrices,

$$\alpha_x = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \alpha_y = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

E. (14) can be decoupled in a set of equations as follows

$$E|\psi_1\rangle = \tilde{c}[p_x + im^*\omega x - ip_y + m^*\omega y]|\psi_2\rangle, \quad (15)$$

$$E|\psi_2\rangle = \tilde{c}[p_x - im^*\omega x + ip_y + m^*\omega y]|\psi_1\rangle, \quad (16)$$

and so, E. (13) reads

$$H_D = \begin{pmatrix} 0 & \tilde{c}[p_x + im^*\omega x - ip_y + m^*\omega y] \\ \tilde{c}[p_x + im^*\omega x - ip_y + m^*\omega y] & 0 \end{pmatrix}. \quad (17)$$

This last form of Hamiltonian of Dirac can be written, in the complex formalism [11, 15, 16], by

$$H_D = \begin{pmatrix} 0 & 2\tilde{c}p_z + im^*\omega\tilde{c}\bar{z} \\ 2\tilde{c}\bar{p}_z - im^*\omega\tilde{c}z & 0 \end{pmatrix}. \quad (18)$$

In this stage, we can see that the form of the Hamiltonian is modified according to the sign of the m^* as follows:

- if $m^* > 0$, the following operators $2\tilde{c}p_z + im^*\omega\tilde{c}\bar{z}$ and $2\tilde{c}\bar{p}_z - im^*\omega\tilde{c}z$ are rewritten with (a_z, \bar{a}_z) couple, defined by E. (7), as

$$2\tilde{c}p_z + im^*\omega\tilde{c}\bar{z} = 2i\tilde{c}^2\sqrt{m^*\omega\hbar}(-i)\left(\frac{1}{\sqrt{m^*\omega\hbar}}p_z + \frac{i}{2}\sqrt{\frac{m^*\omega}{\hbar}}\bar{z}\right) = g\bar{a}_z \quad (19)$$

$$2\tilde{c}\bar{p}_z - im^*\omega\tilde{c}z = -2i\tilde{c}^2\sqrt{m^*\omega\hbar}(i)\left(\frac{1}{\sqrt{m^*\omega\hbar}}\bar{p}_z - \frac{i}{2}\sqrt{\frac{m^*\omega}{\hbar}}z\right) = g^*a_z. \quad (20)$$

So, E. (17) becomes

$$H_D = \begin{pmatrix} 0 & g\bar{a}_z \\ g^*a_z & 0 \end{pmatrix}, \quad (21)$$

with $g = 2im^*\tilde{c}^2\sqrt{r}$ is the coupling strength between orbital and spin degrees of freedom, and $r = \frac{\hbar\omega}{m^*\tilde{c}^2}$ is a parameter which controls the non relativistic limit. According to E. (21), the Dirac Hamiltonian can be written into another form as

$$H_D = g(\sigma^\dagger\bar{a}_z + \sigma^-a_z), \quad (22)$$

and it correspond to the Anti-Jayne's-Cummings (AJC) model.

- if, now, the effective mass $m^* < 0$, the Dirac Hamiltonian becomes

$$H_D = \begin{pmatrix} 0 & 2\tilde{c}p_z - im^{*'}\omega\tilde{c}\bar{z} \\ 2\tilde{c}\bar{p}_z + im^{*'}\omega\tilde{c}z & 0 \end{pmatrix}, \quad (23)$$

with $m^{*'} = -m^* > 0$. By the same way as in the first case, the operators $2cp_z - im\omega'c\bar{z}$ and $2c\bar{p}_z + im\omega'cz$ can be rewritten by

$$2\tilde{c}p_z - im^{*'}\omega\tilde{c}\bar{z} = 2i\tilde{c}\sqrt{m^{*'}\omega\hbar}(-i)\left(\frac{1}{\sqrt{m^{*'}\omega\hbar}}p_z - \frac{i}{2}\sqrt{\frac{m^{*'}\omega}{\hbar}}\bar{z}\right) = ga_{\bar{z}} \quad (24)$$

$$2\tilde{c}\bar{p}_z + im^{*'}\omega\tilde{c}z = -2i\tilde{c}\sqrt{m^{*'}\omega\hbar}(i)\left(\frac{1}{\sqrt{m^{*'}\omega\hbar}}\bar{p}_z + \frac{i}{2}\sqrt{\frac{m^{*'}\omega}{\hbar}}z\right) = g^*\bar{a}_{\bar{z}}, \quad (25)$$

when we have introducing a new creation and annihilation operators $(a_{\bar{z}}, \bar{a}_{\bar{z}})$ couple, defined as follows

$$a_{\bar{z}} = -i\left(\frac{1}{\sqrt{m^{*'}\omega\hbar}}p_z - \frac{i}{2}\sqrt{\frac{m^{*'}\omega}{\hbar}}\bar{z}\right), \quad \bar{a}_{\bar{z}} = i\left(\frac{1}{\sqrt{m^{*'}\omega\hbar}}\bar{p}_z + \frac{i}{2}\sqrt{\frac{m^{*'}\omega}{\hbar}}z\right). \quad (26)$$

Thus, the new form of a Dirac Hamiltonian is

$$H_D = \begin{pmatrix} 0 & g'a_{\bar{z}} \\ g'^*\bar{a}_{\bar{z}} & 0 \end{pmatrix}. \quad (27)$$

Here $g' = 2im^* \tilde{c}^2 \sqrt{r'}$ is the coupling strength between orbital and spin degrees of freedom, and $r' = \frac{\hbar\omega}{m^* \tilde{c}^2}$ is a parameter which controls the non relativistic limit. As above case, E. (27) can be transforms into

$$H_D = g (\sigma^\dagger a_{\bar{z}} + \sigma^- \bar{a}_{\bar{z}}). \quad (28)$$

Here we are in the case of Jayne's-Cummings (JC) model. In both cases $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$ are the spin arising and lowering operators.

We would like mentioned here two remarks: Firstly, the both cases described above are in well agreement with the study of quantum phase transition in the Dirac oscillator performed by Bermudez et al [18]. Secondly, the relativistic Hamiltonian of a two-dimensional Dirac oscillator can be mapped onto a couple of Anti-Jayne's-Cummings and Jayne's-Cummings which describe the interaction between the relativistic spin or and bosons. This mapped between our problem in question and quantum optics using trapped ions is realized experimentally.

Now, Following Esq. (15) and (16), the wave functions ψ_1 and ψ_2 can be rewritten in the language of the complex annihilation-creation operators as

$$|\psi_1\rangle = \frac{g}{E} \bar{a}_z |\psi_2\rangle, \quad (29)$$

$$|\psi_2\rangle = \frac{g^*}{E} a_z |\psi_1\rangle. \quad (30)$$

When we write the component $|\psi_1\rangle$ in terms of the quanta bases, $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle$, these equations can be simultaneously diagonalized, and the energy spectrum can be described by [11]

$$E_n^\pm = \pm \sqrt{4m^* \tilde{c}^2 \hbar \omega n}. \quad (31)$$

Now, when we put that $\omega = \frac{\omega_c}{2}$ with $\omega_c = \frac{eB}{m^*}$ [17] is a classical cyclotron resonance, E. (31) becomes

$$E_n^\pm = \pm \sqrt{2} \frac{\hbar \tilde{c}}{l_B} \sqrt{n}, \quad (32)$$

with $l_B = \sqrt{\frac{\hbar}{eB}}$ is the so-called magnetic length[17]. This definition of the effective mass is consistent with the definition of the cyclotron mass, which is commonly used for experimental measurements of the effective mass. Finally, we apply this definition to graphene and show that it is in agreement with the experimentally observed linear dependence between the

cyclotron mass and momentum[12, 13, 17]. The corresponding total wave function for both positive and negative eigenstates, after normalization, has the following form

$$|\pm E_n\rangle = \begin{bmatrix} \sqrt{\frac{1}{2}}|n\rangle \\ \mp i\sqrt{\frac{1}{2}}|n-1\rangle \end{bmatrix}. \quad (33)$$

Finally, and according to the Esq. (33) and (34), our eigensolutions in the commutative case are in well-agreement with those obtained by [17].

Finally, and according to the results found above, a two dimensional Dirac oscillator can be described graphene under a magnetic field. This means that the last can be mapped onto a couple of anti-Jaynes-Cummings and Jaynes-Cummings models, well known in quantum optics.

Now, by using E. (32), we are able the calculate all thermal properties of graphene, such as such as the free energy, the mean energy, the entropy and the specific heat, have been found by using an approach based on the zeta function.

III. THERMAL PROPERTIES OF GRAPHENE

A. Methods

In order to obtain all thermodynamic quantities of the relativistic harmonic oscillator, we concentrate, at first, on the calculation of the partition function Z . The last is defined by [19]

$$Z = 1 + \sum_{n=0}^{\infty} e^{-\bar{\beta}\sqrt{n}}, \quad (34)$$

where $\bar{\beta} = \frac{1}{\tau}$, and

$$\tau = \frac{l_B}{\sqrt{2}\hbar\tilde{c}} \frac{1}{\beta} = \frac{T}{T_0}, \quad (35)$$

with τ denotes the reduce temperature, and

$$T_0 = \frac{\sqrt{2}\hbar\tilde{c}}{l_B k_B}, \quad (36)$$

is the temperature reference value: when we choose $B = 18\text{T}$, the value of this temperature is

$$T_0 \approx 3551\text{K}. \quad (37)$$

Using the formula (see Ref [20] and references therein)

$$e^{-x} = \frac{1}{2\pi i} \int_C ds x^{-s} \Gamma(s), \quad (38)$$

the sum in E. (34) is transformed into

$$\sum_n e^{-\bar{\beta}\sqrt{n}} = \frac{1}{2\pi i} \int_C ds (\bar{\beta})^{-s} \sum_n n^{-\frac{s}{2}} \Gamma(s) = \frac{1}{2\pi i} \int_C ds (\bar{\beta})^{-s} \zeta\left(\frac{s}{2}\right) \Gamma(s), \quad (39)$$

with $x = \bar{\beta}\sqrt{n}$, and $\Gamma(s)$ and $\zeta\left(\frac{s}{2}\right)$ are respectively the Euler and zeta function. Applying the residues theorem, for the two poles $s = 0$ and $s = 2$, the desired partition function is written down in terms of the Hurwitz zeta function as follows:

$$Z(\tau) = 1 + \tau^2 + \zeta(0). \quad (40)$$

Now, using that $\zeta(0) = \frac{1}{2}$ the final partition function is transformed into

$$Z(\tau) = \tau^2 + \frac{1}{2}. \quad (41)$$

From this definition, all thermal properties of our system, such as the free energy, the entropy, total energy and the specific heat, can be obtained through the numerical partition function $Z(\tau)$ via the following relations [19]

$$\bar{F} = \frac{l_B}{\sqrt{2\hbar\tilde{c}}} F = -\frac{1}{\bar{\beta}} \ln(Z) = -\tau \ln(Z), \bar{U} = \frac{l_B}{\sqrt{2\hbar\tilde{c}}} U = -\frac{\partial \ln(Z)}{\partial \bar{\beta}} = \tau^2 \frac{\partial \ln(Z)}{\partial \tau}, \quad (42)$$

$$\bar{S} = \frac{S}{k_B} = \bar{\beta}^2 \frac{\partial \bar{F}}{\partial \bar{\beta}} = \ln(Z) + \tau \frac{\partial \ln(Z)}{\partial \tau}, \bar{C} = \frac{C}{k_B} = -\bar{\beta}^2 \frac{\partial \bar{U}}{\partial \bar{\beta}} = 2\tau \frac{\partial \ln(Z)}{\partial \tau} + \tau^2 \frac{\partial^2 \ln(Z)}{\partial \tau^2}. \quad (43)$$

B. Numerical results and discussions

The thermodynamic quantities are, respectively, plotted in Figures. 1,2,3 and 4. Before discussing the main results, we discuss the behavior of the specific heat in the asymptotic regions, i.e, in the regimes of the higher temperature: in this region, the partition function can be approximated by

$$Z(\tau) \simeq \tau^2,$$

which yields to the following results

$$\bar{U} = 2\tau,$$

$$\bar{C} = 2.$$

We can argue this by saying that these limits follow the Dulong-Petit law for an ultra-relativistic ideal gas[19].

Now, we are ready to present our numerical results for all thermal properties of graphene under an uniform magnetic field obtained via our model based on a two-dimensional Dirac oscillator: we should mention that, in all the figures, we have used adimensional quantities; and all thermal quantities are plotted versus a reduce temperature τ .

In Fig. 1, we depicted the free energy versus a reduce temperature τ : we can see that it decreases with a temperature as expected. From Fig. 2, we can see that the total energy increases with the temperature, and has a linear behavior in higher temperatures regime. Concerning the entropy function (Fig. 3), we observe that it increases with temperature without showing an abrupt change in its form. That allows us to explain that the curvature, observed in the specific heat curve (Fig. 4), does not exhibit or indicate an existence of a phase transition around a $\tau_0 = 1.5$. This value of τ_0 is different with that found by [19].

Recently, Sanstos et al [19] have studied the thermodynamics properties of graphene in non commutative phase-space. They obtained all thermodynamics quantities by using the Euler-MacLaurin approximation. We note here, that first, it is not clear why the authors used E. (10) instead E. (7) in their calculations. Also, the formalism used by the authors seems to have the following problems: (i) the existence of the remains term (Esq. (20) and (21) in Ref [19]) makes that the calculations become difficult to find, and (ii) the partition function diverges when $\tau \rightarrow 0$.

Finally, we can see that the thermal properties of graphene can be obtained easily with the approach based on zeta function than the formalism of Euler-MacLaurin. Also, we found that our system can be mapped with quantum optics: the quantum optics theory provides one of the first testing grounds for the application of the open quantum systems. The theory of open quantum systems addresses the problems of damping and dephasing in quantum systems by its assertion that all real systems of interest are in fact “open” systems, each surrounded by its environment. Therefore, and following these arguments, the system of graphene can be regarded as an appropriate scenario of the theory of an open quantum systems coupled to a thermal bath (see Ref. [11] and references therein).

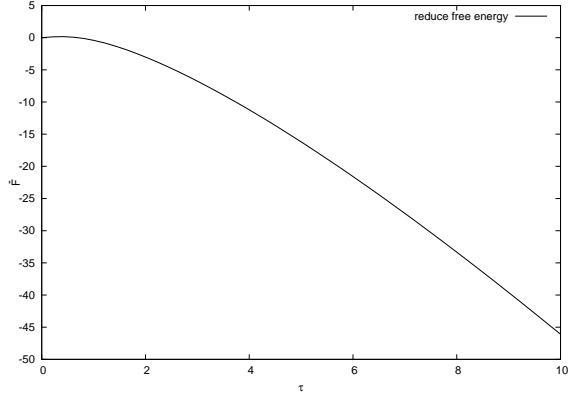


Figure 1. The reduce free energy \bar{F} versus a reduce temperature τ .

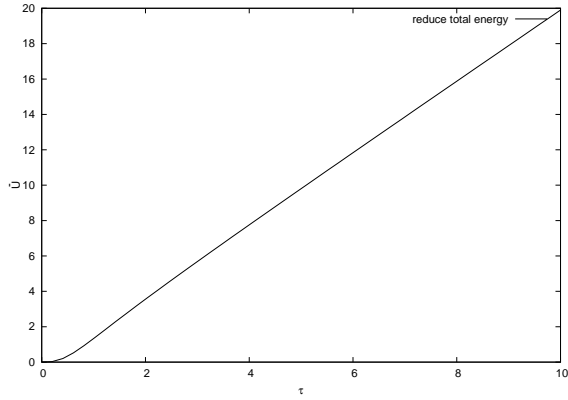


Figure 2. The reduce total energy \bar{U} versus a reduce temperature τ .

IV. CONCLUSION

In the present work, we have shown that the formalism of the effective mass in graphene allowed us to find the eigensolutions of the last by using the model based on Dirac oscillator interaction. All thermodynamic properties of graphene have been determined using an approach based on the zeta function method.

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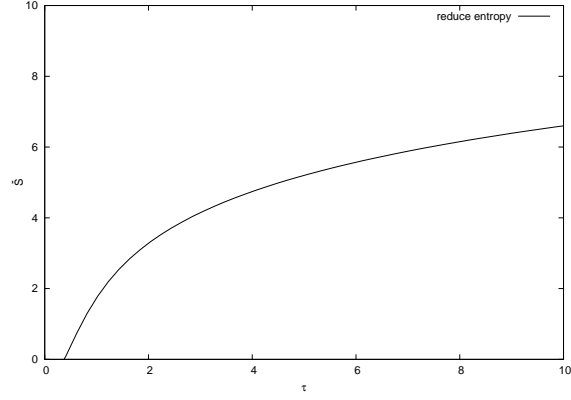


Figure 3. The reduce entropy function \bar{S} versus a reduce temperature τ .

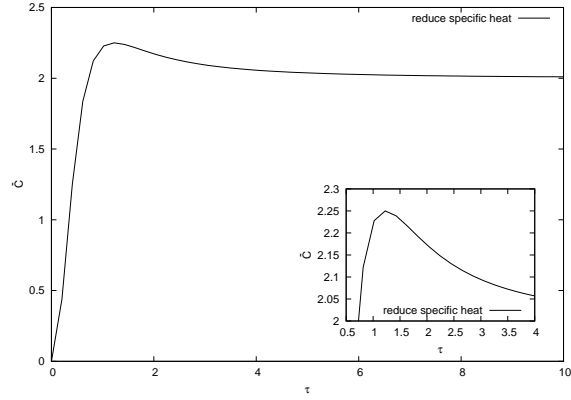


Figure 4. The reduce specific heat \bar{C} versus a reduce temperature τ .

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